

Checking Out the Hot Spots

WHEN a high-explosive material detonates, several events happen virtually instantaneously. A shock wave slams into the material, compresses it with pressures up to 400,000 times that of Earth's atmosphere, and causes it to release chemical energy, which heats it to over 3,500°C. The heat releases power approaching 10 billion watts per square centimeter to sustain the shock wave, which travels as fast as 10 kilometers a second. All of these reactions occur within less than a millionth of a second.

High explosives are an essential component of a nuclear weapon because they initiate the nuclear reaction. The study of high explosives has been an integral part of nuclear weapons research for Livermore scientists since 1952, when the Laboratory began operations. However, it has been a challenge for the scientists to find avenues for observing exactly what happens during high-explosive detonations, given the speed and extreme conditions in which they happen.

The National Nuclear Security Administration's (NNSA's) Stockpile Stewardship Program, which began in 1994, placed emphasis on another aspect of high-explosive research. Because the program's mission is to ensure the safety of the nation's nuclear stockpile without underground testing, Livermore weapon scientists focused their research on how high-explosive material may change in an aging stockpiled nuclear weapon.

A crucial part of high-explosive research is the study of voids, or defects, in high-explosive material. Normally, a defect is seen as something that makes a material less than perfect. But voids in high explosives are an important part of the ignition process, because they enable the material to explode. Voids are small pockets—usually between 1 to 20 micrometers in size—either filled with air or, in some cases, a byproduct gas of the surrounding crystalline high-explosive grains or polymer binder. During the detonation process, the shock wave deforms and compresses the material, which then engulfs the area occupied by the voids. What remains are hot spots—small isolated regions of high explosive at a much higher temperature than the surrounding material. These hot spots are where ignition of the high explosive begins.



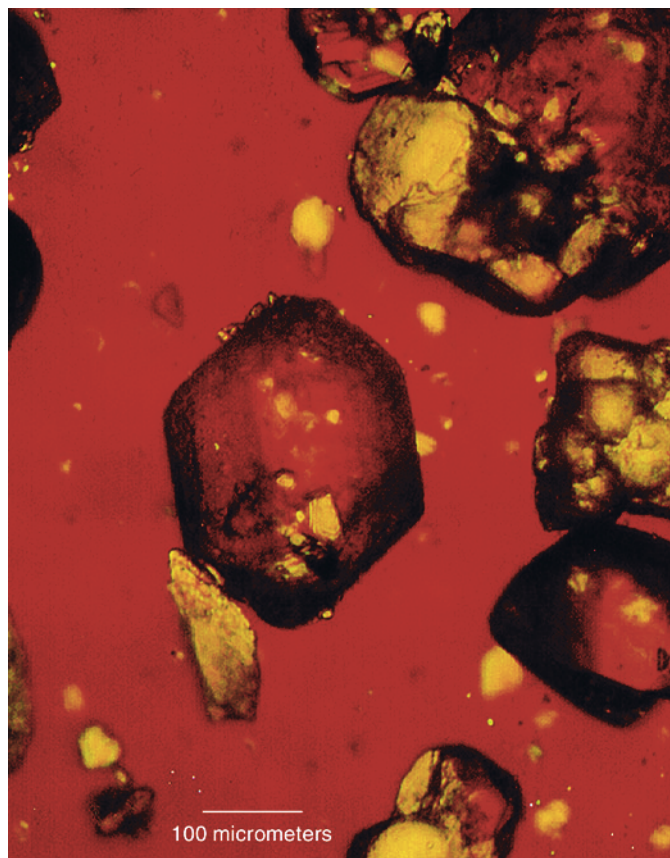
A Long History

The research involving voids is a study of balance. Material with too few voids will result in too few hot spots, making ignition difficult. In addition, if hot spots are too small, they will cool prematurely, preventing ignition. But high explosives with too many voids can be too sensitive and explode from mishandling.

Investigating the role of hot spots in explosives has never been easy. Historically, scientists relied on rules of thumb in materials science, laboratory testing of explosives, and accident analysis to determine the dynamics of explosive materials. All of these methods are time- and labor-intensive.

In early experiments, scientists crushed a piece of explosive material on a glass plate and identified small spots of light seen from underneath as hot spots. Eventually, their research capabilities expanded, and they began using simple computational models. The early models were limited, however, because they treated the explosive as a homogeneous material. High explosives are anything but. They are composed of various constituents and can include one or more crystalline components, plastic binders, and voids.

The chemistry that occurs in a detonation can also be complex. For example, 300 different reactions can occur when the high-explosive material tetranitro tetraazacyclooctane (HMX) detonates. Depending on the circumstances of combustion, each reaction can involve different pathways. Models developed at Livermore in the 1970s were based on this realization but needed considerable experimental calibration.

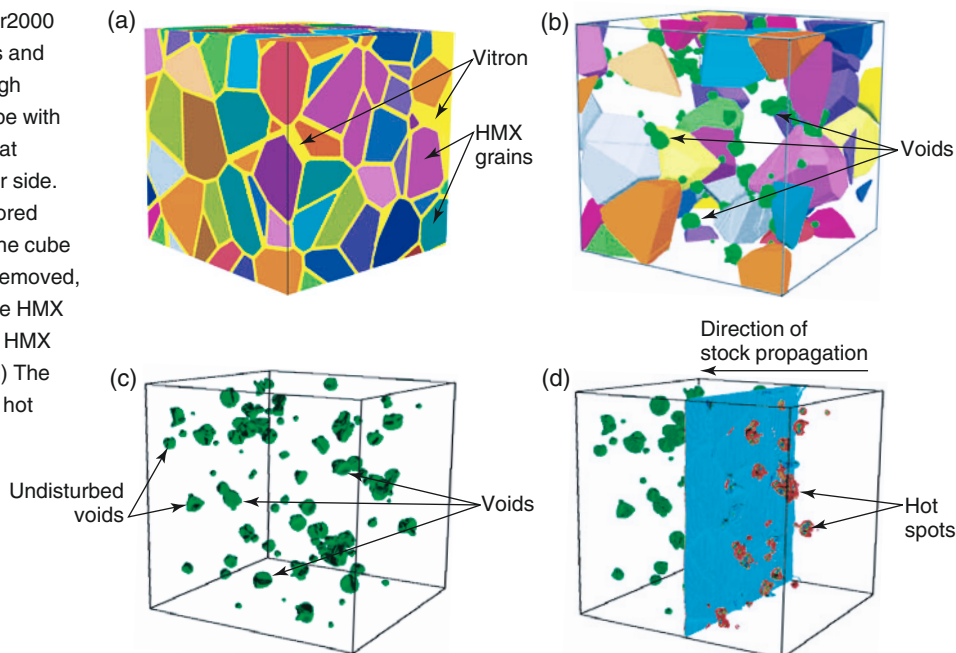


Defects, or voids, are a necessary component in a high explosive because they cause the material to ignite. This photomicrograph shows defects in a 150-micrometer HMX crystal.

With the development of supercomputers, scientists have the capability to simulate high-explosive detonation and, in particular, observe hot spots in action. “The importance of hot spots in explosive materials has been known since the 1940s,” says computational physicist Jack Reaugh. “Until recently, however, observing hot spots in detail has been extremely difficult.” For several years now, Reaugh has been studying hot spots and voids using hydrodynamic computational codes, which describe material flow under extreme pressures. (See *S&TR*, June 1999, pp. 12–18.) In his first simulation in 1999, Reaugh designed a cube with 36 HMX particles, each 0.05 millimeter in size. He then simulated the detonation of the cube on a computer workstation using ALE3D, a three-dimensional computational code developed at Livermore.

In the fall of 2001, Reaugh, with the help of physicist Stew Keeton, took advantage of Livermore’s new TeraCluster2000 (TC2K) supercomputer and ran a new simulation, again with ALE3D and using 128 of the TC2K’s processors for 500 computing hours. This time, the cube contained a more complex combination of simulated HMX. The cube measured 100 micrometers per side—about the diameter of a human hair—and contained about 100 grains of HMX represented by various geometric shapes, along with a light-colored fluorocarbon polymer binder between the grains. Voids were inserted into the cube so that they made up 1 percent of its volume. The simulation generated a shock wave that swept across the cube. It hit the material at 120,000 times Earth’s atmospheric pressure at sea level. The compression collapsed the voids and transformed them into isolated hot spots with temperatures of over 900 kelvins—100 to 200 kelvins higher than the surrounding material.

This simulation, performed on the TeraCluster2000 supercomputer, tracked the evolution of voids and resulting hot spots during detonation of the high explosive HMX. (a) The simulation uses a cube with approximately 100 grains of high explosive that measures approximately 100 micrometers per side. The shaded grains are HMX and the light-colored veins are a polymer binder called Vitron. (b) The cube with the binder and some of the HMX grains removed, so that the voids, located between some of the HMX grains, are visible. (c) The cube with all of the HMX and binder removed, showing all the voids. (d) The shock wave moves through the cube, leaving hot spots where the voids used to be.



Refining the Model

"The sequence of events revealed in the TC2K simulation showed how important supercomputer capabilities are to this field of study," Reaugh says. As in most new work, the first attempt gave Reaugh some ideas on how to improve the model for the next simulation. "A big portion of this project is just designing the model," he continues, "and each pass improves it." He could see, for example, that the simulated HMX crystals were too big and that he needed to change the chemical reaction rates and transport properties.

Through an effort funded under the joint Department of Defense–Department of Energy Munitions Technology Development Program, Reaugh collaborated with Livermore scientists whose experimental work gauged Reaugh's results. Part of Reaugh's work focuses on how flames propagate between hot spots and how propagation speed affects the response of the explosive to high-pressure shocks. For the TC2K simulation, Reaugh estimated the distance between the hot spots based on his calculations of flame speed at high pressure. Meanwhile, chemist Joe Zaug and his colleagues used the high pressures of a diamond anvil cell for HMX experiments in which they measured propagation speeds at over 300,000 atmospheres. The experiments showed the flame speed to be up to 100 times faster than Reaugh initially calculated for the simulation. "This meant that the hot spots could have been 100 times farther apart than I originally thought," Reaugh says.

At the same time, theoretical chemist Riad Manaa performed quantum molecular dynamics calculations—that is, calculations of the interactions between atoms and electrons—to determine the rate of chemical decomposition of HMX at high temperature and pressure. "When we compared results, Manaa's calculations showed the decomposition to be happening much faster than we thought. In fact, his rates are almost fast enough to account for the difference between our estimate of the flame speed and Zaug's measurements," notes Reaugh.

The differences pointed out that additional capabilities were needed in the computational code. "We were able to see things that needed to be improved with ALE3D so that it could deal gracefully with some very stressing calculations that we're planning for the future."

Building on these observations, Reaugh's group ran a new simulation in September 2002. The simulation was performed on Livermore's most powerful supercomputer, ASCI White, part of NNSA's Advanced Simulation and Computing (ASCI) Program. The new model cube was designed for optimum use of ASCI White and incorporated lessons learned from the previous simulation. Again, HMX was used. The variety of grain sizes was increased dramatically. Voids amounting to 2 percent of the volume were inserted into the explosive grains. The new cube measured approximately 300 micrometers per side and contained 93,000 grains, quite a jump from the 100 grains used in the



Improvements to the simulation were tested in September 2002. The simulation used a new cube that consisted of approximately 93,000 grains of different shapes and sizes. Voids shaped like spheres were inserted into the grains. This simulation also incorporated improvements to the equations of state for explosive products and the chemical reaction kinetics models.

previous simulation. Just generating the initial cube assembly took 400 processors about 4 computing hours. By reducing the level of detail but retaining the distribution of voids, engineer Tom Reitter and Reaugh, with the help of computer support associate Estella McGuire, were able to simulate the propagation of a shock wave through a brick consisting of four cubes stacked end to end. That simulation took less than 100 hours and showed the shock wave speeding up as reactions behind the shock front built up pressure. "This simulation never could have been done without the computational power that we have now," Reaugh says.

Details of a Larger Picture

With the powerful supercomputers and codes now available, scientists can simulate high-explosive detonations in sufficient detail to observe detonation behavior under a multitude of parameters. "Whereas before, we had to rely on piecemeal data from tests," notes Reaugh, "now, the details of ASCI simulations help us to interpret what went on in the experiment."

Because the simulations will also help scientists understand how high explosives respond during manufacturing, shipping, and storage, they will not only benefit the Stockpile Stewardship Program but also help the high-explosives industry.

The study of explosive materials is at once becoming more comprehensive and more focused.

—Laurie Powers

Key Words: ALE3D, Advanced Simulation and Computing (ASCI) Program, chemical kinetics, high explosives, high-pressure activities, hot spots, HMX, hydrodynamics codes, TeraCluster2000 (TC2K), voids.

For further information contact Jack Reaugh (925) 422-7206 (reaugh1@llnl.gov).